Mass Spectral Interpretation - Tips and Tools for GC-EI-MS and High-Resolution MS Data

November 15, 2022 | 9:00am- 4:00pm

Host: Edward Sisco & Arun Moorthy

Description: Mass spectrometry is one of the most commonly employed analytical tools in forensic chemistry disciplines. While many users employ large mass spectral databases for interpretation, there are use cases where more in-depth analysis is required (*e.g.* new psychoactive substances that are not present in a database). This workshop will provide attendees with tips and tricks for mass spectral interpretation as well as demonstrate some of the tools that are available from NIST to further assist chemists in interpreting spectra. This workshop will emphasize data obtained from gas chromatography electron ionization mass spectrometry (GC-EI-MS), but ambient ionization high-resolution mass spectrometry data will also be discussed.

Agenda:

9:00 - 9:20 Introductory remarks - Edward Sisco

9:20 – 10:00 NIST Mass Spectral Libraries & Tools Overview – Arun Moorthy

10:00 – 10:45 Case Study #1 (Traditional Sample Analysis) – Edward Erisman

10:45 - 11:00 Break

11:00 – 11:45 Case Study #2 (Tackling Co-elution) – Gary Mallard

11:45 - 1:00 Lunch

1:00 – 1:45 Case Study #3 (Elucidating an Unknown) – James Little

1:45 – 2:30 Case Study #4 (Elucidating an Unknown) – David Sparkman

2:30 - 2:45 Break

2:45 - 4:00 Open Discussion - All